



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 1, 2026 – 10:32 am BST

PDB ID : 29UQ / pdb_000029uq
Title : KAT6A SURFACE MUTANT IN COMPLEX WITH CO-FACTOR
ACETYL-CO-A
Authors : Hillig, R.C.; Puetter, V.
Deposited on : 2026-04-09
Resolution : 2.13 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

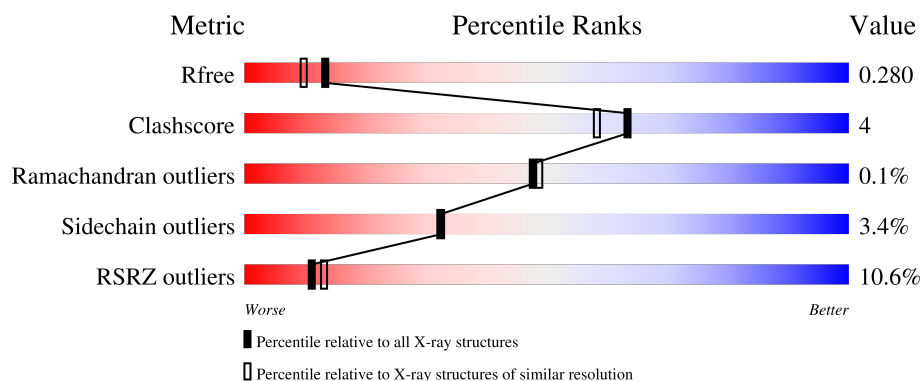
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	272	 6% 89% 10% ..
1	BBB	272	 18% 89% 10% .
1	CCC	272	 12% 86% 12% ..
1	DDD	272	 6% 88% 11% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone acetyltransferase KAT6A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	270	Total	C	N	O	S	0	5	0
			2290	1485	391	401	13			
1	BBB	269	Total	C	N	O	S	0	5	0
			2267	1473	381	400	13			
1	CCC	267	Total	C	N	O	S	0	6	0
			2264	1471	380	400	13			
1	DDD	269	Total	C	N	O	S	0	3	0
			2260	1467	380	399	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	507	GLY	-	expression tag	UNP Q92794
AAA	508	SER	-	expression tag	UNP Q92794
AAA	638	SER	CYS	engineered mutation	UNP Q92794
AAA	646	SER	CYS	engineered mutation	UNP Q92794
AAA	723	SER	CYS	engineered mutation	UNP Q92794
AAA	773	SER	CYS	engineered mutation	UNP Q92794
BBB	507	GLY	-	expression tag	UNP Q92794
BBB	508	SER	-	expression tag	UNP Q92794
BBB	638	SER	CYS	engineered mutation	UNP Q92794
BBB	646	SER	CYS	engineered mutation	UNP Q92794
BBB	723	SER	CYS	engineered mutation	UNP Q92794
BBB	773	SER	CYS	engineered mutation	UNP Q92794
CCC	507	GLY	-	expression tag	UNP Q92794
CCC	508	SER	-	expression tag	UNP Q92794
CCC	638	SER	CYS	engineered mutation	UNP Q92794
CCC	646	SER	CYS	engineered mutation	UNP Q92794
CCC	723	SER	CYS	engineered mutation	UNP Q92794
CCC	773	SER	CYS	engineered mutation	UNP Q92794
DDD	507	GLY	-	expression tag	UNP Q92794
DDD	508	SER	-	expression tag	UNP Q92794
DDD	638	SER	CYS	engineered mutation	UNP Q92794

Continued on next page...

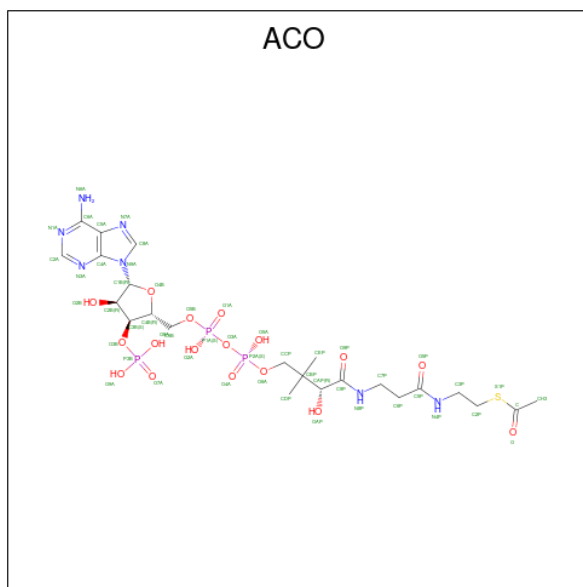
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	646	SER	CYS	engineered mutation	UNP Q92794
DDD	723	SER	CYS	engineered mutation	UNP Q92794
DDD	773	SER	CYS	engineered mutation	UNP Q92794

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Zn	0	0
			1	1		
2	BBB	1	Total	Zn	0	0
			1	1		
2	CCC	1	Total	Zn	0	0
			1	1		
2	DDD	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



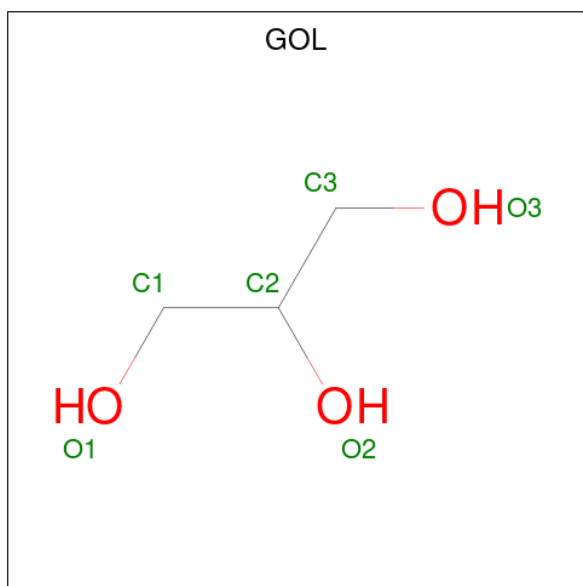
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	BBB	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	CCC	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

Continued on next page...

Continued from previous page...

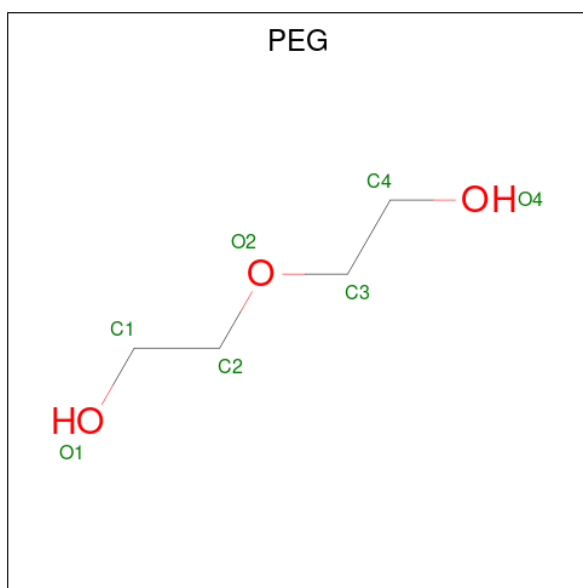
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	DDD	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	BBB	1	Total	C	O	0	0
			6	3	3		
4	BBB	1	Total	C	O	0	0
			6	3	3		
4	CCC	1	Total	C	O	0	0
			6	3	3		
4	CCC	1	Total	C	O	0	0
			6	3	3		
4	CCC	1	Total	C	O	0	0
			6	3	3		
4	DDD	1	Total	C	O	0	0
			6	3	3		
4	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	DDD	1	Total	C	O	0	0
			7	4	3		

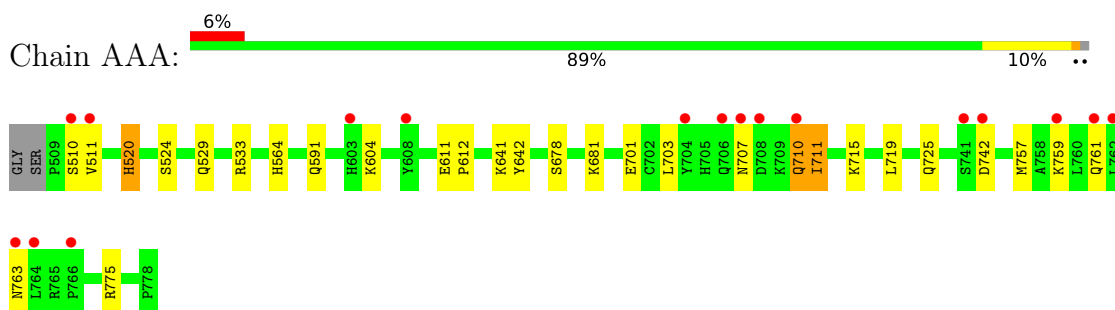
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	185	Total	O	0	0
			185	185		
6	BBB	128	Total	O	0	0
			128	128		
6	CCC	148	Total	O	0	0
			148	148		
6	DDD	169	Total	O	0	0
			169	169		

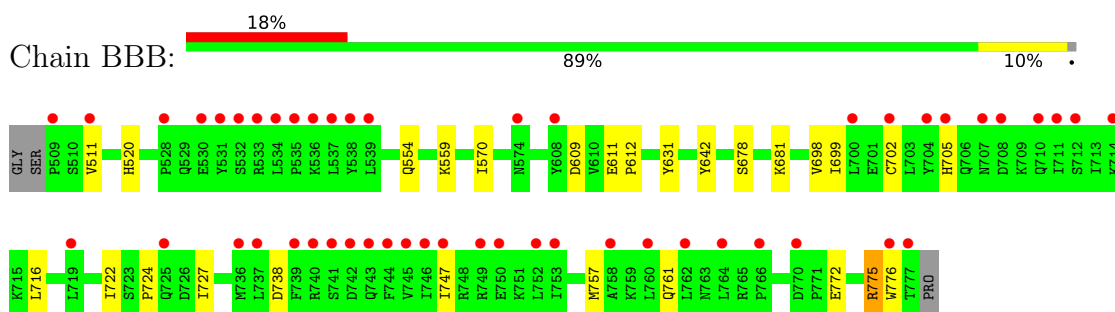
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

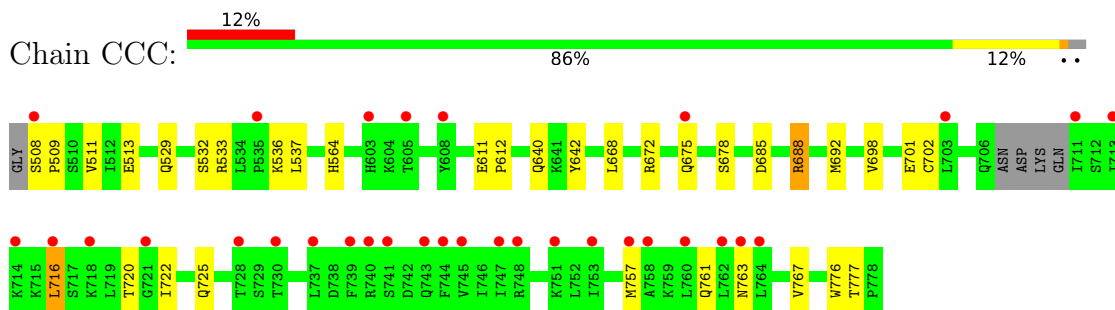
- Molecule 1: Histone acetyltransferase KAT6A



- Molecule 1: Histone acetyltransferase KAT6A

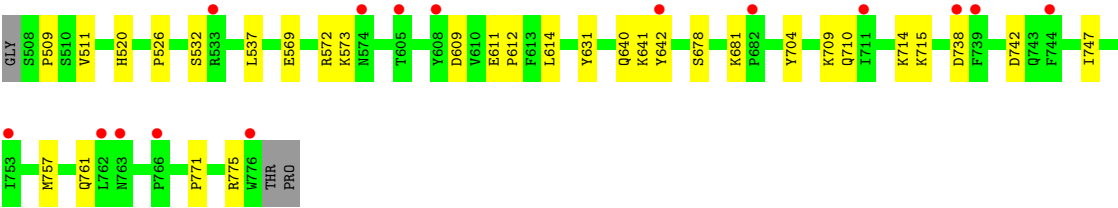


- Molecule 1: Histone acetyltransferase KAT6A



- Molecule 1: Histone acetyltransferase KAT6A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.30Å 64.59Å 115.62Å 85.61° 85.18° 89.61°	Depositor
Resolution (Å)	44.59 – 2.13 44.59 – 2.13	Depositor EDS
% Data completeness (in resolution range)	90.7 (44.59-2.13) 90.7 (44.59-2.13)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.275 0.230 , 0.280	Depositor DCC
R_{free} test set	2100 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9986	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3316e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACO, ALY, PEG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	1.01	1/2355 (0.0%)	1.32	0/3176
1	BBB	1.03	0/2328	1.35	0/3143
1	CCC	1.01	1/2333 (0.0%)	1.32	1/3148 (0.0%)
1	DDD	1.04	0/2317	1.35	0/3127
All	All	1.02	2/9333 (0.0%)	1.33	1/12594 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	564	HIS	CE1-NE2	5.54	1.38	1.32
1	AAA	564	HIS	CE1-NE2	5.45	1.38	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	777	THR	CB-CA-C	5.02	115.39	109.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2290	0	2308	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	2267	0	2273	16	0
1	CCC	2264	0	2282	22	0
1	DDD	2260	0	2271	17	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	51	0	34	0	0
3	BBB	51	0	34	0	0
3	CCC	51	0	34	0	0
3	DDD	51	0	34	0	0
4	AAA	18	0	24	0	0
4	BBB	12	0	16	0	0
4	CCC	18	0	24	1	0
4	DDD	12	0	16	1	0
5	DDD	7	0	10	2	0
6	AAA	185	0	0	6	0
6	BBB	128	0	0	1	0
6	CCC	148	0	0	0	0
6	DDD	169	0	0	2	0
All	All	9986	0	9360	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 74 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:715:LYS:O	1:AAA:719:LEU:HD12	1.74	0.87
1:BBB:716:LEU:HD23	1:BBB:727[B]:ILE:HD11	1.55	0.85
1:AAA:711:ILE:H	1:AAA:711:ILE:HD13	1.46	0.80
1:BBB:698:VAL:HG21	1:BBB:722:ILE:HD11	1.70	0.74
1:AAA:725:GLN:HG3	6:AAA:1019:HOH:O	1.89	0.72

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	272/272 (100%)	265 (97%)	6 (2%)	1 (0%)	30	26
1	BBB	271/272 (100%)	261 (96%)	10 (4%)	0	100	100
1	CCC	269/272 (99%)	265 (98%)	4 (2%)	0	100	100
1	DDD	269/272 (99%)	261 (97%)	8 (3%)	0	100	100
All	All	1081/1088 (99%)	1052 (97%)	28 (3%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	707	ASN

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	258/254 (102%)	247 (96%)	11 (4%)	26	23
1	BBB	255/254 (100%)	245 (96%)	10 (4%)	28	26
1	CCC	257/254 (101%)	251 (98%)	6 (2%)	44	47
1	DDD	255/254 (100%)	243 (95%)	12 (5%)	23	19
All	All	1025/1016 (101%)	986 (96%)	39 (4%)	32	28

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	520	HIS
1	DDD	709	LYS
1	DDD	532[A]	SER
1	DDD	640	GLN
1	DDD	771	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	ALY	BBB	604	1	10,11,12	0.41	0	7,12,14	0.29	0
1	ALY	CCC	604	1	10,11,12	0.41	0	7,12,14	0.35	0
1	ALY	AAA	604	1	10,11,12	0.39	0	7,12,14	0.38	0
1	ALY	DDD	604	1	10,11,12	0.38	0	7,12,14	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	BBB	604	1	-	1/9/10/12	-
1	ALY	CCC	604	1	-	1/9/10/12	-
1	ALY	AAA	604	1	-	1/9/10/12	-
1	ALY	DDD	604	1	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	CCC	604	ALY	C-CA-CB-CG
1	AAA	604	ALY	C-CA-CB-CG
1	BBB	604	ALY	C-CA-CB-CG
1	DDD	604	ALY	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	604	ALY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	AAA	805	-	5,5,5	0.11	0	5,5,5	0.26	0
4	GOL	BBB	803	-	5,5,5	0.09	0	5,5,5	0.31	0
3	ACO	CCC	802	-	48,53,53	0.50	1 (2%)	69,79,79	0.59	0
3	ACO	DDD	802	-	48,53,53	0.41	0	69,79,79	0.58	0
4	GOL	AAA	803	-	5,5,5	0.12	0	5,5,5	0.31	0
4	GOL	CCC	805	-	5,5,5	0.15	0	5,5,5	0.28	0
4	GOL	BBB	804	-	5,5,5	0.11	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACO	BBB	802	-	48,53,53	0.41	0	69,79,79	0.59	0
4	GOL	CCC	803	-	5,5,5	0.13	0	5,5,5	0.34	0
4	GOL	DDD	804	-	5,5,5	0.10	0	5,5,5	0.26	0
3	ACO	AAA	802	-	48,53,53	0.45	0	69,79,79	0.61	0
4	GOL	DDD	803	-	5,5,5	0.10	0	5,5,5	0.30	0
5	PEG	DDD	805	-	6,6,6	0.21	0	5,5,5	0.15	0
4	GOL	AAA	804	-	5,5,5	0.11	0	5,5,5	0.34	0
4	GOL	CCC	804	-	5,5,5	0.11	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	AAA	805	-	-	0/4/4/4	-
4	GOL	BBB	803	-	-	2/4/4/4	-
3	ACO	CCC	802	-	-	2/51/67/67	0/3/3/3
3	ACO	DDD	802	-	-	2/51/67/67	0/3/3/3
4	GOL	AAA	803	-	-	2/4/4/4	-
4	GOL	CCC	805	-	-	2/4/4/4	-
4	GOL	BBB	804	-	-	2/4/4/4	-
3	ACO	BBB	802	-	-	3/51/67/67	0/3/3/3
4	GOL	CCC	803	-	-	2/4/4/4	-
4	GOL	DDD	804	-	-	0/4/4/4	-
3	ACO	AAA	802	-	-	1/51/67/67	0/3/3/3
4	GOL	DDD	803	-	-	4/4/4/4	-
5	PEG	DDD	805	-	-	1/4/4/4	-
4	GOL	AAA	804	-	-	2/4/4/4	-
4	GOL	CCC	804	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	802	ACO	P3B-O3B	2.06	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	803	GOL	O1-C1-C2-C3
4	BBB	804	GOL	C1-C2-C3-O3
4	CCC	803	GOL	C1-C2-C3-O3
4	CCC	805	GOL	C1-C2-C3-O3
5	DDD	805	PEG	O1-C1-C2-O2

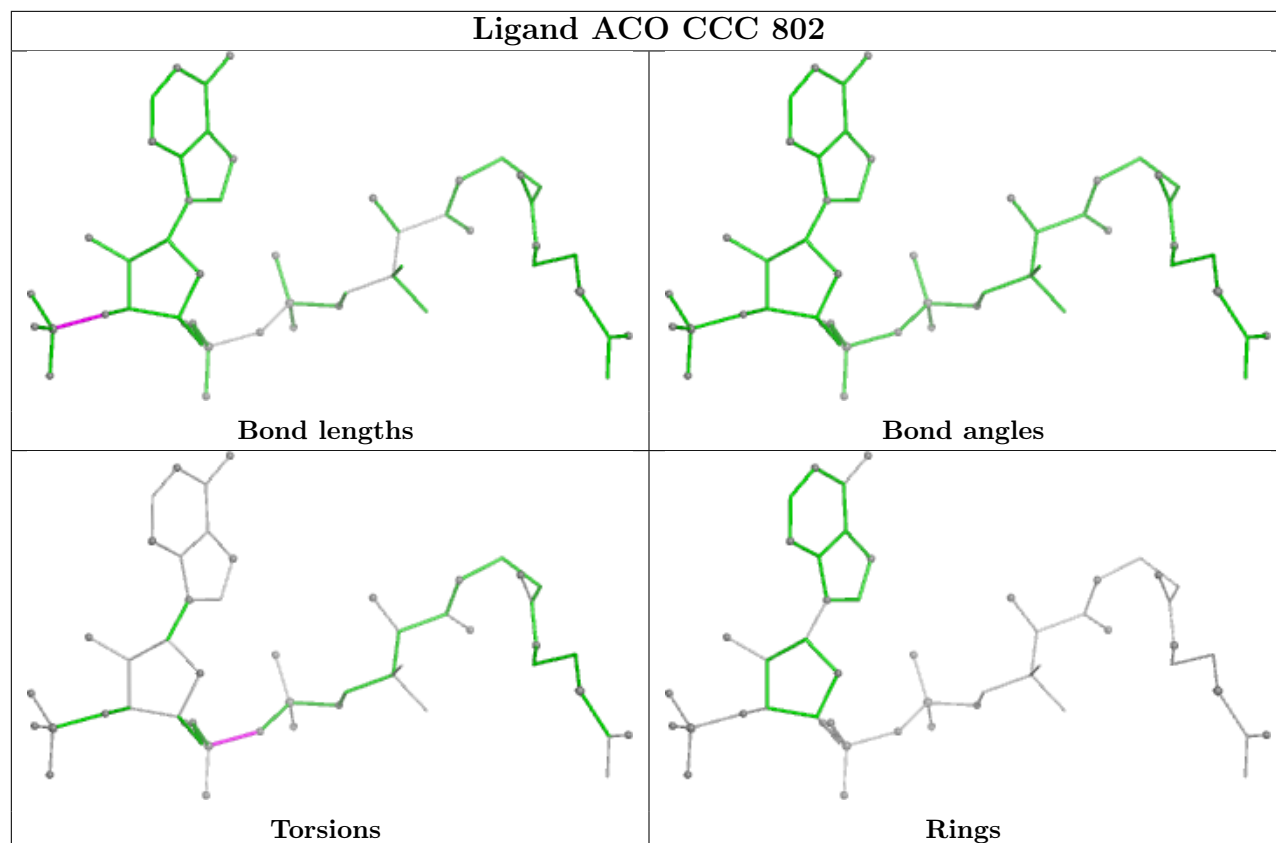
There are no ring outliers.

3 monomers are involved in 4 short contacts:

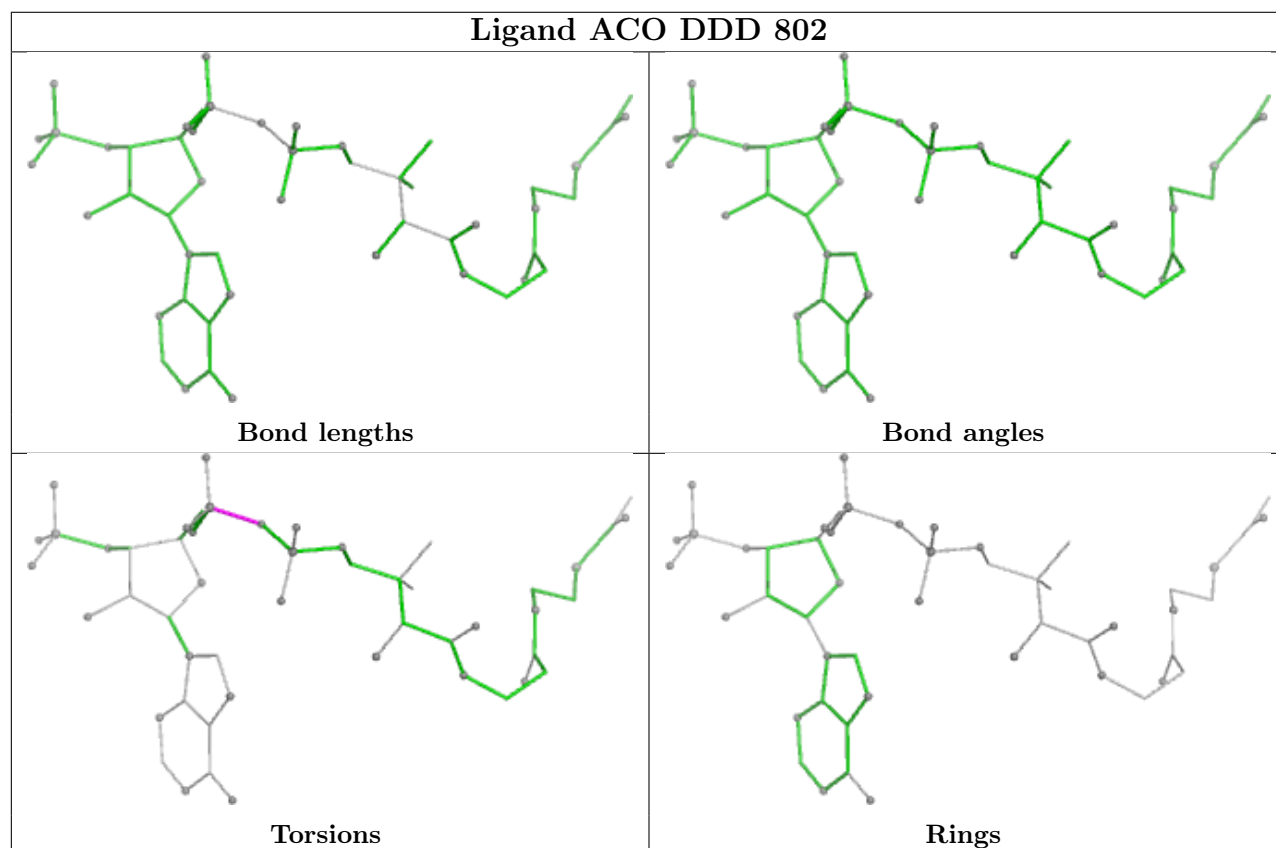
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	803	GOL	1	0
5	DDD	805	PEG	2	0
4	CCC	804	GOL	1	0

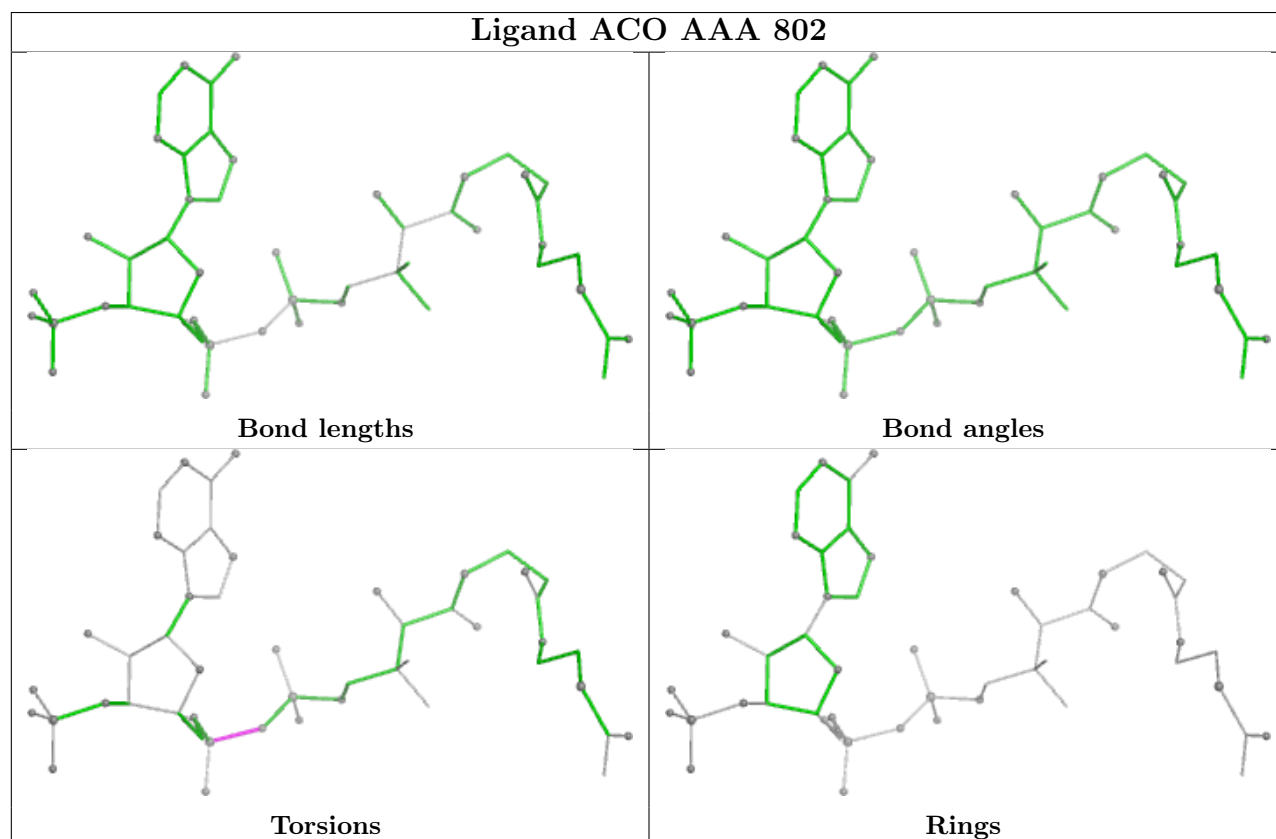
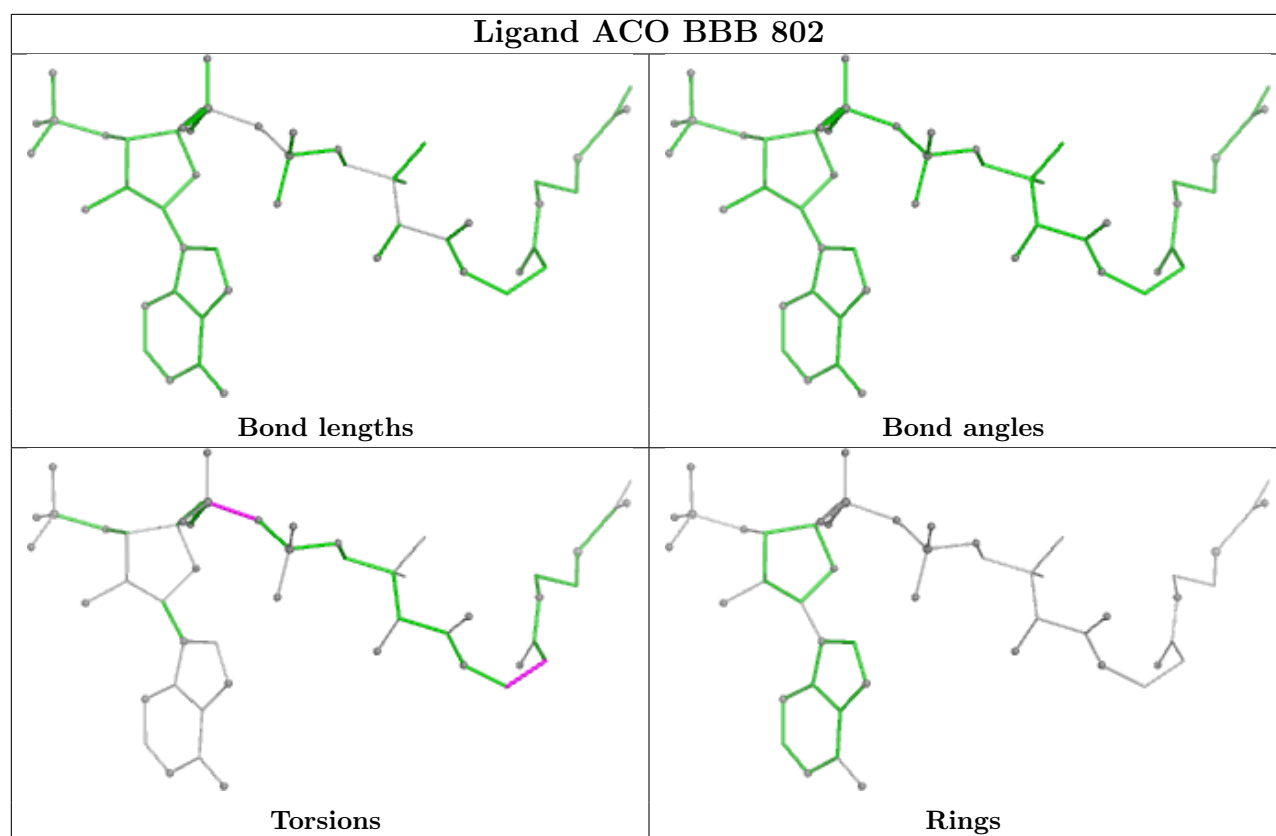
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ACO CCC 802



Ligand ACO DDD 802





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	269/272 (98%)	0.48	17 (6%) 26 30	15, 28, 53, 88	5 (1%)
1	BBB	268/272 (98%)	1.17	50 (18%) 3 4	23, 41, 95, 132	5 (1%)
1	CCC	266/272 (97%)	0.79	32 (12%) 9 10	19, 35, 83, 117	6 (2%)
1	DDD	268/272 (98%)	0.66	15 (5%) 30 34	16, 31, 55, 78	3 (1%)
All	All	1071/1088 (98%)	0.78	114 (10%) 11 13	15, 33, 81, 132	19 (1%)

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	535	PRO	5.1
1	DDD	762	LEU	4.9
1	BBB	708	ASP	4.8
1	BBB	533	ARG	4.6
1	CCC	739	PHE	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	ALY	DDD	604	12/13	0.89	0.10	24,28,34,34	0
1	ALY	CCC	604	12/13	0.90	0.10	28,32,43,43	0
1	ALY	BBB	604	12/13	0.92	0.10	27,30,36,37	0
1	ALY	AAA	604	12/13	0.95	0.08	22,24,30,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

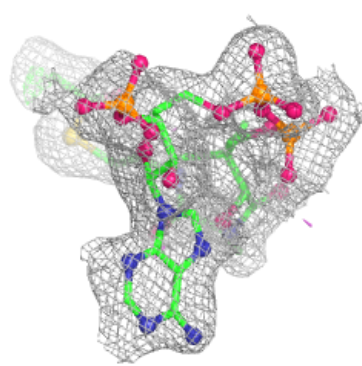
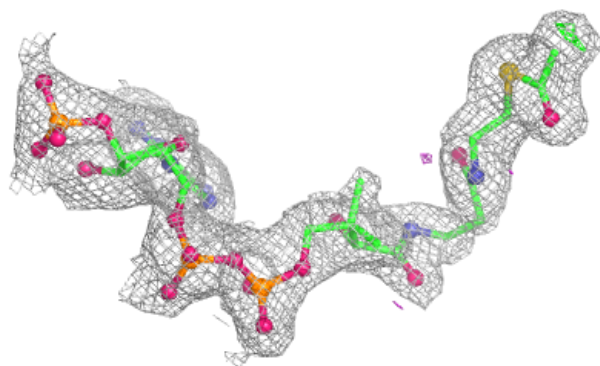
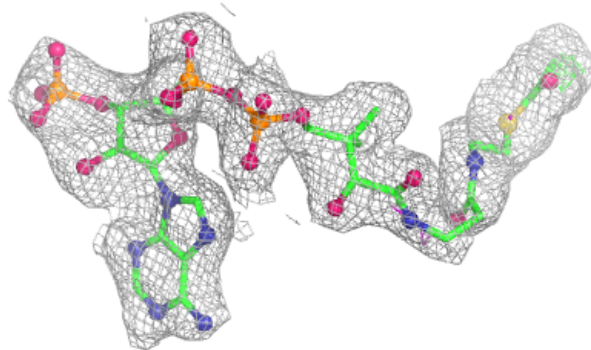
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	DDD	805	7/7	0.71	0.17	43,52,62,68	0
4	GOL	CCC	803	6/6	0.72	0.16	49,51,54,54	0
4	GOL	BBB	803	6/6	0.74	0.19	43,46,47,51	0
4	GOL	AAA	803	6/6	0.79	0.12	44,45,52,55	0
4	GOL	DDD	803	6/6	0.82	0.12	43,46,54,61	0
4	GOL	BBB	804	6/6	0.84	0.13	32,38,47,57	0
4	GOL	AAA	804	6/6	0.87	0.11	43,44,47,55	0
4	GOL	CCC	805	6/6	0.88	0.10	21,23,26,32	0
4	GOL	CCC	804	6/6	0.89	0.17	22,26,36,53	0
4	GOL	AAA	805	6/6	0.90	0.10	25,34,42,44	0
4	GOL	DDD	804	6/6	0.91	0.10	28,37,45,49	0
3	ACO	BBB	802	51/51	0.91	0.10	22,34,49,57	0
3	ACO	AAA	802	51/51	0.93	0.09	16,27,37,39	0
3	ACO	DDD	802	51/51	0.94	0.08	13,23,36,49	0
3	ACO	CCC	802	51/51	0.94	0.08	17,29,43,45	0
2	ZN	BBB	801	1/1	0.95	0.06	22,22,22,22	0
2	ZN	AAA	801	1/1	0.96	0.05	23,23,23,23	0
2	ZN	CCC	801	1/1	0.96	0.09	21,21,21,21	0
2	ZN	DDD	801	1/1	0.96	0.07	22,22,22,22	0

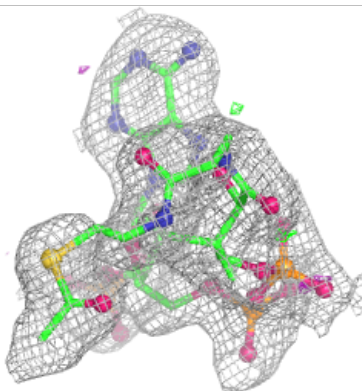
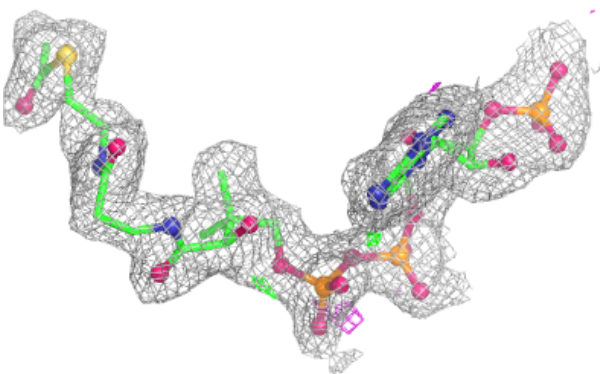
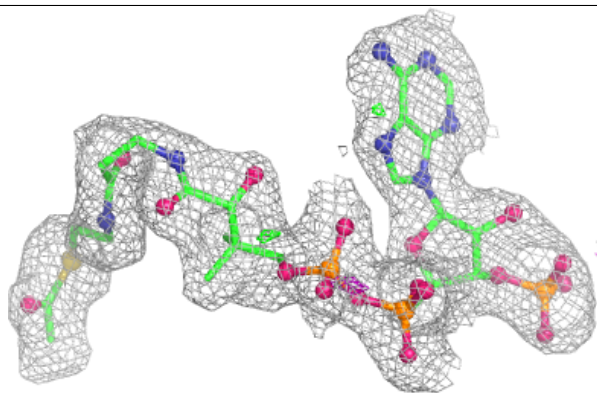
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ACO BBB 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

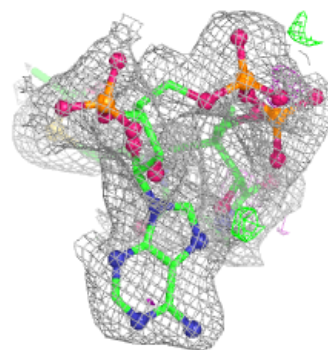
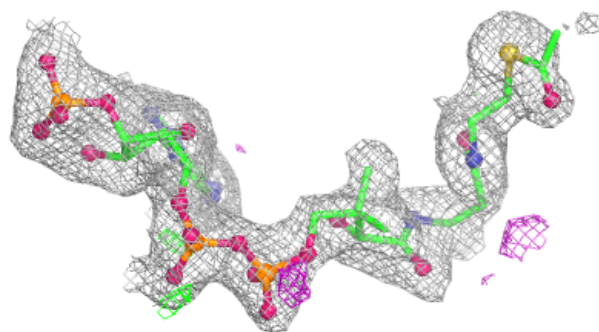
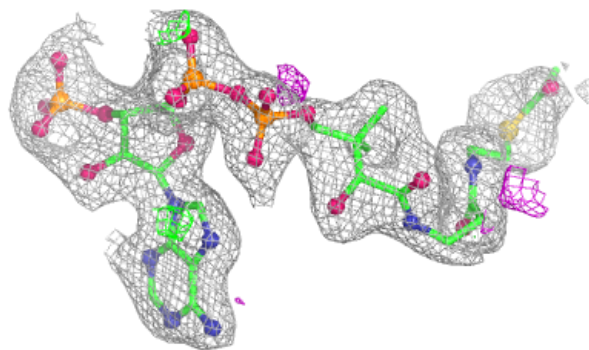
**Electron density around ACO AAA 802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

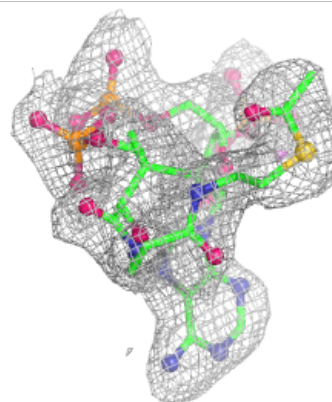
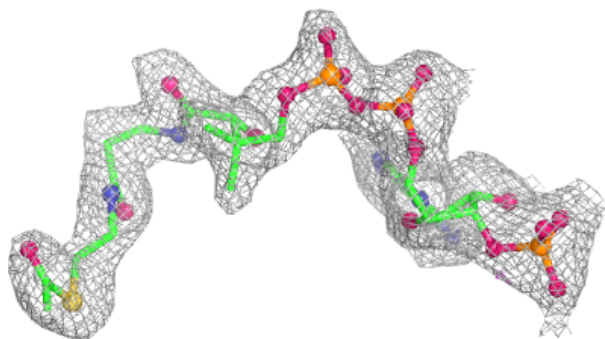
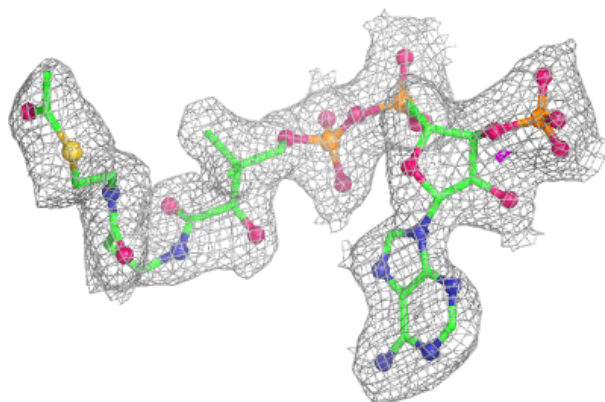


Electron density around ACO DDD 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ACO CCC 802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.